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PROGRESS REPORT 1 JANUARY 1981 - 31 DECEMBER 1982
COMPUTER INSTALLATION

Abstract. This report describes selected parts of the activities at the Computer Installation of Risø National Laboratory in 1981 and 1982. Information given may be preliminary.

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CONTENTS

	Page
1. INTRODUCTION	5
2. THE COMPUTER INSTALLATION, 1981-1982	6
3. THE NEW COMPUTER BUILDING	8
3.1. A Bit of History	8
3.2. Description of the Building	9
4. CHANGING A CENTRAL COMPUTER INSTALLATION IN LESS THAN 24 HOURS	12
5. FORTRAN 77 ON B7800	16
5.1. Fortran 77 Test Project 1981-1982	16
5.2. Problems with Linkage Software	17
5.3. Visit to Burroughs in Paoli, USA	18
5.4. Completion of Benchmarking and Status Ultimo 1982	19
6. WORKING ENVIRONMENT AND SECURITY	21
7. LIBRARY	23
8. RECENT DEVELOPMENT IN RISØ COMPUTER LIBRARY	25
9. RISØ INTERACTIVE PLOTTING SYSTEM	26
9.1. RIPS as a Library	26
9.2. RIPS in Fortran	27
10. THE TEXT-EDITING SYSTEM SETUP	28
11. REDUCE - AN ALGEBRAIC PROGRAMMING SYSTEM IMPLEMENTED ON RISØ'S B7800 COMPUTER	29
12. IMPROVED DISKALLOCATION ALGORITHM	31

	Page
13. DIVISION OF COMPLEX NUMBERS	33
14. TRAINING ACTIVITIES	35
15. FORMATION CONSTANTS IN CHEMICAL EQUILIBRIUM REACTIONS	37
16. MATHEMATICAL MODEL FOR ATMOSPHERIC TURBULENCE	39
17. USERPROGRAMMER	41
18. SCANNET'S CONNECTION TO B7800	43
19. MULTIPLE QUADRATURE	45
APPENDIX A. CONFIGURATION OF THE RISØ B7800 COMPUTER AS OF DECEMBER 1982	46
APPENDIX B. STAFF OF THE COMPUTER INSTALLATION 1 JANUARY 81 - 31 DECEMBER 82	49
APPENDIX C. PRODUCTION STATISTICS 1981	50
APPENDIX D. PRODUCTION STATISTICS 1982	51
APPENDIX E. B6700 STATISTICS, 1971-1982	52

1. INTRODUCTION

This report describes selected activities at the Computer Installation of Risø National Laboratory in 1981 and 1982.

During these two years there has been a total change in the physical environment of our work as the former Burroughs B6700 computer has been replaced by a B7800 which was installed in a new building with a computer room, technical installations for heat removal, stores, and reception area for the users.

Following a short survey of the period this report tells about the new building, the change of computer, our work with Fortran 77, which was closely connected with the B7800, and about considerations for the working environment.

Next follow chapters which describe activities of value to the user community on the whole. This includes work with the Library concept in Burroughs basic software, The Risø Computer Library, the graphical RIPS software, text editing, and the algebraic language Reduce. Improvements in allocation of disk storage and in the routine for complex division are mentioned here as well as our educational effort.

In the last part we discuss assistance to specific users, primarily construction of mathematical models for chemical and meteorological problems. Also, the connection of our computer to the Scandinavian research datanet, Scannet, is treated.

Finally, an appendix gives operational statistics and lists of staff and equipment. As the B6700 now has been closed down after nearly twelve years' service, we print the graphs of monthly processor time and aggregated Cande terminal connect time since the machine log system and the Cande systems became operational in April 1971, and May 1974, respectively.

2. THE COMPUTER INSTALLATION, 1981-1982

In early 1981 we were still evaluating proposals and benchmarks for a new computer. On 25 March 1981 management decided to negotiate a contract with Burroughs on a B7800. The contract was concluded with 1 July 1982 as the date when the computer should have passed Risø's acceptance test.

An important part of the contract concerned the availability of a Fortran 77 system, which will be imperative in Risø's future work. In 1981, the Burroughs Fortran 77 was only in the development state and this led to a close cooperative effort between us and Burroughs, which is described at length in a later chapter in this report.

The remaining part of 1981 and spring 1982 was mainly used in preparing for the new computer, including the planning and erection of a new building, and for developing course material and giving a large number of courses to the users.

Installation of the B7800 began in May 1982. Acceptance test with full load of users ran from 17-30 June 1982, on the evening of which date the acceptance document was signed; however, the Fortran 77 was approved only in December.

We suffered from a severe lack of computing capacity during the last half year with the B6700, although it was run in three shifts. This situation was effectively remedied when the B7800 took over, as it is nearly eight times faster on the average, and so far it can easily provide the capacity during the hours when the users want it available.

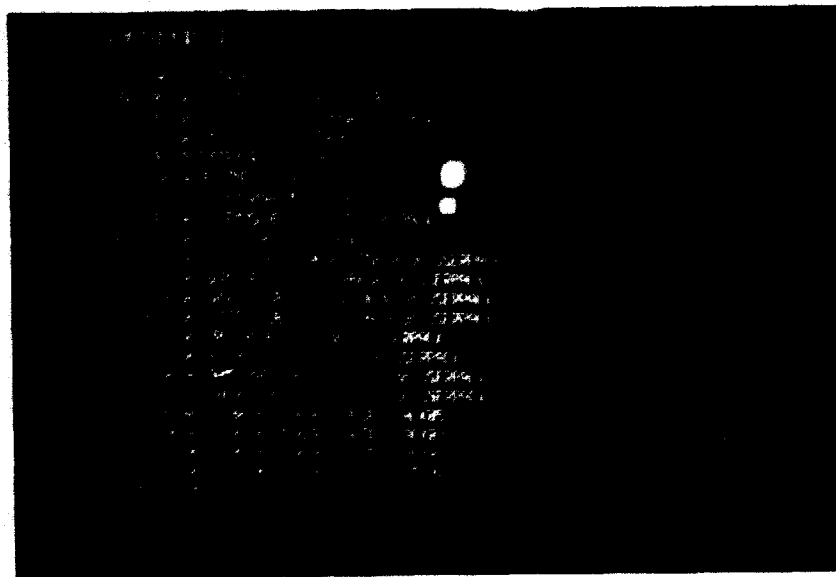
B6700's ports for interactive terminals were permanently overloaded in the daytime, and the buying of more terminals was actively discouraged.

Nevertheless, there has been a strong growth in the use of terminals. Whereas the total connect time at the beginning of the period was about 1600 hours each month, at the end it had grown to about 2500 hours. At the same time, the number of terminals in the departments was nearing 90, and the number of terminal adapters in the B7800 had also grown above expectations.

A new structure of the terminal network is being considered at the end of the report period.

The terminal equipment for the staff of the Computer Installation was augmented by three VDU terminals; furthermore three old terminals were replaced because the keyboards were worn out and unreliable. The Diablo printer, which is used for text processing, is in heavy use, and an extra Diablo 1650 KSR terminal was bought at the end of the period.

After the B6700 was removed, the whole building was refitted, and the Computer Installation's terminals, self-service line-printer, and punch machines were moved to refitted rooms next to the new computer building.



List of active entities in B7800, shown on the operator's console

3. THE NEW COMPUTER BUILDING

3.1. A Bit of History

When it had been decided to replace the old B6700 with a B7800, the next question that arose was where to place the new computer.

Twelve years ago, the B6700 had been installed in a standard Risø laboratory building, a solution which had worked out but never been fully satisfactory, and it was certainly not acceptable by 1982 standards.

The main problems were that the computer room was long and narrow, available space for air-conditioning was inadequate, there were no fire protection partitions, and there was no practical way to enforce the access control that the Danish Public Authorities' Act of 1978 called for.

It would be both very expensive and time consuming to build an acceptable computer room in an existing building. Further, if it should be done in the B6700 room, it would necessarily mean a break for several months in the computer service, removing the B6700, rebuilding with fire protection and new technical installations, and installing and testing out the B7800. Use of other rooms would mean a re-housing problem for their present users.

So, it was decided to erect a new building to house the new computer. After the inevitable compromises between wishes and financial realities, its size was fixed to 450 m² on one floor. It was placed next to the building that housed the B6700.

The new building consists of the computer room, library for magnetic tapes and diskpacks, store for paper and similar utilities, air-conditioning to keep temperature and humidity constant, the field engineers' shop, job reception and output delivery room,

operation and advisory service, and sanitary facilities. A plan of the building is shown on the next page.

Unfortunately, the technical conditions (temperature, humidity, different methods of air intake into different units, the free height below the floor, number of transformers) were changed by the computer vendor during the design of the building. Further drama arose from an extremely cold and snowy winter and from the bankruptcy of the main-contractor during the construction phase. Nevertheless, the building was ready on the scheduled date, 1 May 1982.

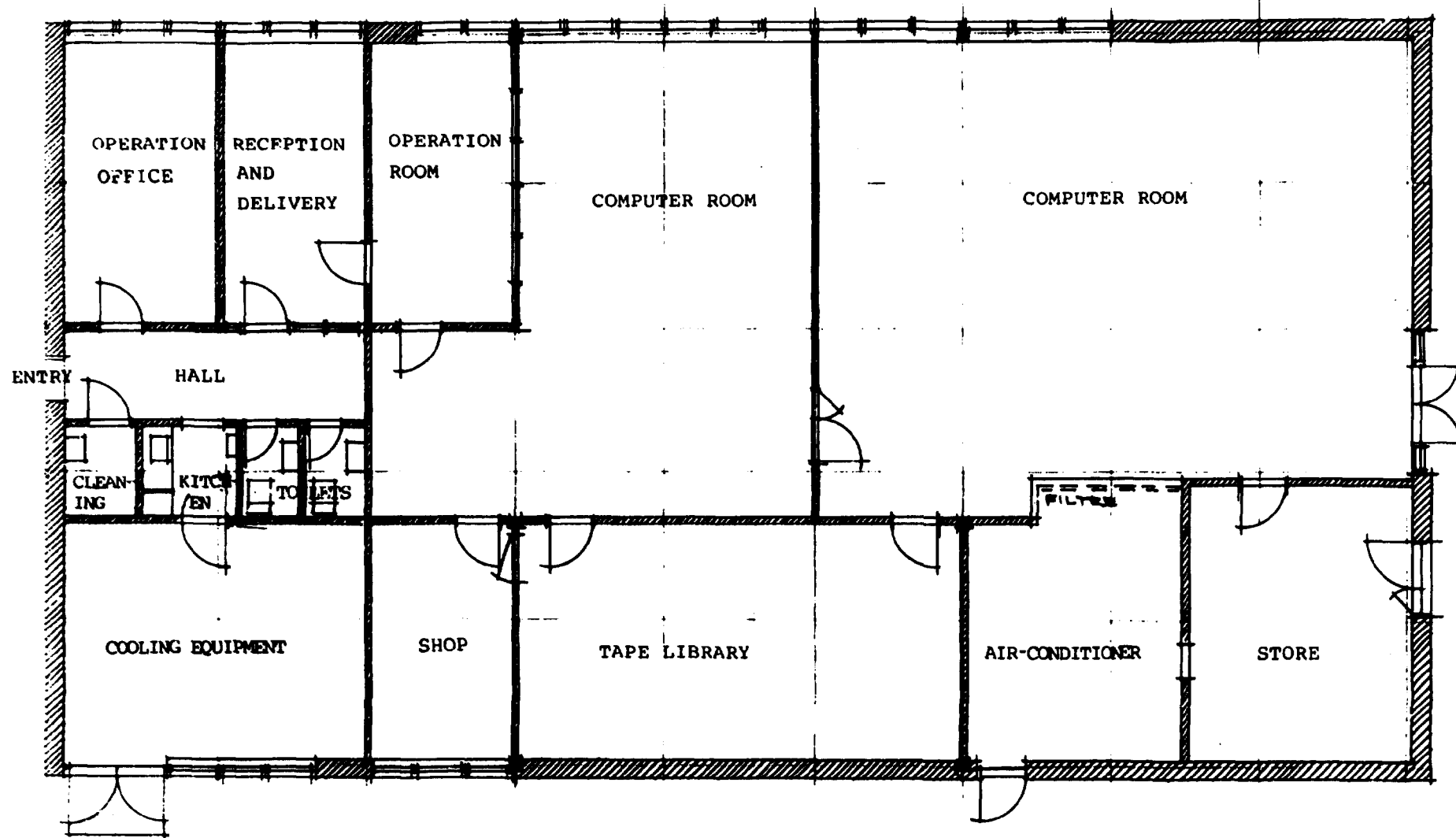
3.2. Description of the Building

The computer room itself has been divided into two rooms. Line-printer, magnetic tape drives, and digital plotters are in one room of 60 m², while units which do not need frequent handling are gathered in the other one of 120 m².

Both rooms are cooled by air of 15 °C using the space under the floor as a plenumduct. The air is exhausted from the room through a filter in the wall. When the computer is switched off, the air flow is automatically reduced to half so that the room temperature is kept at 22 °C. If need be, the air is moistened to give a relative humidity between 40 and 60%.

The air is cooled by two cooling batteries with water at minimum 11 °C, and the water is again cooled by two cooling plants using Freon 12. The water circuit includes a 5 m³ buffer tank. When the actual demand for cooling is changed, the temperature of the circulating water is correspondingly regulated. Depending upon the season, the waste heat from the compressor is either exchanged to the outside air, or is used to heat an office building.

The cooling system was designed by Risø's Engineering Department.



Acoustic noise from fans and ventilation is attenuated by rows of baffles under the ceiling. There is also attenuation material below the floor. The operator consoles are put in the operations room, from where you can look into the first computer room and keep an eye upon magnetic tape stations and digital plotters through windows made of glass of low sound transmission.

The computer room and the tape library are protected against fire by two separate Halon 1301 systems. In the event of an alarm from the ion detectors, Halon will automatically be released into the relevant rooms, including the space below the false floor, and presumably will extinguish the fire.

The lay-out of the building is such that there is only one normal entrance to the computer room, and that is through the operations room. This gives the necessary access control. Other doors, windows, and walls are protected by alarms, and so is the door to the operations room outside working hours.

As the users no longer have access to the computer room, a self-service lineprinter, a Centronics 6080, has been installed outside the protected area.

The decision to erect a new building for the specific purpose of housing the central computer has made it possible to reach suitable solutions within the given economic constraints.

4. CHANGING A CENTRAL COMPUTER INSTALLATION IN LESS THAN 24 HOURS

In 1981 it was decided to substitute the central computer, an 11 years old Burroughs B6700, by a dual processor Burroughs B7800, which is currently the most powerful computer in the series of Burroughs Large Systems.

On 1 May 1982 the new building was ready to receive the B7800. The parts of the new computer were shipped from different plants in USA, and they arrived in several consignments in early May.

During the installation of the B7800 a very dramatic incident occurred while the central processors were unloaded from the truck that brought the hardware to Risø. When the first processor cabinet was taken out of the truck to the plate of the hydraulic lift, the lift could not carry the weight, because of a fault in the hydraulic system. The lift dropped suddenly so that the processor cabinet was at an angle threatening to tilt and fall to the ground. Fortunately, one of the transport workers was still in the truck with his belts fastened to the cabinet. And he was able to hold it back until the other transport workers got control of the situation, and lifted the processor cabinet back into the truck. After loading the processor cabinets into another truck with the defect lift supported by the lift of the first truck, unloading of the processors proceeded without further complications.

It was a part of the contract that drives for diskpacks and magnetic tape units should be carried over from the B6700 to the B7800 and that Burroughs would supply us with extra units for the installation period. The extra units were installed on B6700 and the permanent units were moved to B7800, so that the transfer had minimal implications for the users.

In parallel with the preparations and installations of the hardware, the software for the B7800 was available from Burroughs already in April 1982.

One major factor in the preparation of the software was that Burroughs Large Systems run on basically the same software, and that Large Systems are even code compatible. This means that a program compiled on the B6700 will execute correctly on the B7800, though recompilation may involve performance improvements on the B7800. Similarly, the software for the B7800 could be checked out and compiled on the B6700.

We had stressed emphasis on the availability of the same software release for the B7800 as the current release in operation on the B6700. Unfortunately, the software releases were not fully synchronised at the time of installation, so we had to invest more effort in preparing the software than expected.

Despite this extra effort, we were ready to move the work of generating the software to B7800 from the first day the new computer was able to do useful work.

From that moment the final hardware and software installations were performed in parallel. As soon as the software was installed several test programs were run to verify results by comparison with similar results from the B6700.

The B6700 had a number of terminals connected to it, about 20 via Risø's internal telephone exchange and modems, and a half dozen which had separate connections.

To minimize disturbance in terminal service, all telephone lines were connected in parallel to both the B6700 and B7800, so that a call would be answered by the computer which had the modem at the time being. New cables were laid and connected directly to the appropriate terminals.

All terminals to the B7800 were verified one by one with minimal disturbance to the users. Testing of modem-connected lines was

hardly noticeable as they were removed from the usual chain of numbers. In case of separate connections, the plug into the terminal was changed after prior notice while the tests were carried out.

The verification and test period also had a purpose in verifying the stability of the new system.

When the system had proven its stability, we announced both the B6700 and the B7800 closed from 8 a.m. on 16 June until 9 a.m. 17 June.

During this day all remaining jobs in the B6700 were run and all user files dumped to back-up tapes. Then the total library of 3000 magnetic tapes was moved to the new premises together with diskpacks, modems, plotters, shelves for output, and other items. Plugs for terminals were exchanged and user software libraries loaded on the B7800 to reproduce the closing-down status of the B6700.

The most optimistic users logged on the B7800 at 2 p.m. on 16 June, and they did not experience any difference from running on the B6700 except for a considerable gain in computer power.

The B6700 was turned off permanently, and upgrading to B7800 was complete and successful.

A half dozen software errors showed up on the B7800. Most were solved in a couple of days. The only one of these errors that lasted concerned the Pascal compiler, which was impossible to run because of some differences between the two versions of the basic software. The compiler was a university product which had been available for a short time on our B6700, and no user was severely hurt because of its malfunction. Burroughs is expected to provide a new Pascal compiler soon, and this matter is laid to rest until then.

The acceptance test of B7800 ran for ten working days, where the availability of the system must be above 98%. The test period was successfully concluded on 30 June.

About a month later we had a rough time when some chips became intermittently unreliable, but by September 1982 the situation became stable.



A look into the Central Processor Unit of the B7800

5. FORTRAN 77 ON B7800

In 1978 Fortran 77 was approved as the current American standard for Fortran. This so-called ANSI standard is prescribed in detail in the document ANSI X3.9-1978. In 1980 Fortran 77 also became the European Standard (ISO). Fortran 77 replaces the old standard from 1966, frequently referred to as 'Fortran IV' or 'Fortran 66'. Important language upgradings are the new character data type and use of structural (if-then-else) program elements.

5.1. Fortran 77 Test Project 1981-1982

From the fall of 1981 and throughout 1982 The Computer Installation has been heavily involved in test and debugging work with the Fortran 77 software of Burroughs. The background for this was the requirements to the compiler and its performance laid down in the Contract of Sale for B7800 in 1981. These specifications were negotiated with Burroughs mainly on the initiative of Ole Gunneskov, Risø Engineering Department, and Peter Kirkegaard, Computer Installation, who felt that a good deal of work had to be done by Burroughs before an acceptable Fortran 77 system could be offered to Risø's users. Risø was to prepare a batch of benchmark programs which Burroughs would guarantee to run correctly under Fortran 77 by the time of installation for B7800 in the summer of 1982. Running times were not allowed to exceed the corresponding Fortran 66 times by more than 20%.

In the selection of benchmark programs we considered it important to verify that Risø codes written in Fortran 66 - maybe after minor adaptations - could run under Burroughs' Fortran 77. Four codes or code systems were chosen with a combined length of 60 000 lines.

By a modest effort from Risø these programs were adjusted to comply with the Fortran 77 standard. Burroughs informed us that we could have a Fortran 77 compiler operational at B6700 from about August 1981, but in fact it was installed only in November 1981 for test at the Computer Installation, first for compilations only, and from January 1982, after a new version was installed, also for execution of code.

The process of getting the programs running under Fortran 77 took place as a joint activity of Risø and Burroughs, using B6700 and later B7800: Detailed knowledge of the programs enabled Risø to localize compiler bugs, isolate them in mini-programs (typically of 10 lines each), and promptly hand these to Burroughs as error documentation. Our early experience with the compiler was certainly not encouraging. We detected numerous bugs, some quite serious, both on compile time and on run time. Up to the end of 1982 we have reported about 50 errors. Therefore, in the initial phase, progress in the work was slow, though the situation became significantly better later on.

In the early versions of the Fortran 77 compiler, both compilation and runtime efficiencies were disappointing. In June 1982, the compiler software was sufficiently consolidated to permit the running of the three first benchmark programs. The results obtained were correct, and the running efficiency was roughly the same as with Fortran 66. Not surprisingly, it turned out that the fourth and largest program, Adina, was by far the most taxing. Several compiler errors prevented the successful execution of all the test jobs; and for those data sets which actually could run, execution times were a factor 2 - 10 larger than with Fortran 66. For this reason, the Fortran 77 software could not be taken over by Risø at the B7800 delivery date.

5.2. Problems with Linkage Software

Special problems occurred in connection with the linkage facilities available with Burroughs Fortran 77. The important point here is that Burroughs does not intend to implement the Autobind

facility with Fortran 77; this device allowed the modification of subroutines without a need for total recompilation, and it also made a flexible linkage of library subroutines to Fortran programs possible. Instead Burroughs offers two different pieces of software to replace the function of the Binder in conjunction with Fortran 77: Makehost/Sepcomp for separate compilation of subprograms when updating large programs, and the so-called Library facility. Medio 1982 Sepcomp suffered from several errors and was virtually useless. Use of a Fortran 66 compiled Library from Fortran 77 should be possible in principle but was not in practice due to a compiler error. Production of a Library from Fortran 77 was scheduled but not yet implemented. And the Library had at least two serious drawbacks that violate common Fortran practice and impede the practical use of Fortran libraries at Risø: 1) a dummy argument of a Library routine cannot itself be a procedure, and 2) the user must supply "skeleton routines" to access the library. Thus the Fortran programmer will definitely experience Library as a step backwards compared to Autobind.

5.3. Visit to Burroughs in Paoli, USA

The above mentioned problems and errors were discussed with the Burroughs Compiler Group during a two-day visit to Paoli in October 1982.

At that time Risø had written an analysis report on the work done hitherto: "Fortran 77 on B7800: A Benchmark Analysis", by Peter Kirkegaard and Ole Gunneskov (Computer Installation Memo No. 48, September 1982.) The people in the compiler group were surprised that Risø had had unsolved Fortran 77 problems for such a long time, and they suggested that there was poor communication somewhere in the Burroughs organization. In the future, we were welcome to use a more informal contact directly to the group alongside the official channels. During the first day all of Risø's pending error reports were checked against the current software in Paoli (Mk. 3.4 prerelease.) It turned out

that a significant improvement in the compiler status had taken place relative to Risø's version: 12 errors had disappeared. A few errors still remained unsolved. One bug was fixed the same day.

Also the problems with linkage software were discussed. Concerning Sepcomp, a major error clean-up and rewriting had taken place recently. The status of Library was less encouraging. They pointed out that this software was outside the realm of the Compiler Group and we agreed that the best thing Risø could do with the Library problems was to exercise pressure at the highest possible level and as often as possible.

A variety of other problems were also discussed. They were on the borderline between errors and inadequate design. Typical issues in this category were aspects of filehandling, which is not fully standardized by ANSI, possible improvements in the layout of list-directed output, and the complex division operator (this is a common system routine, which is discussed elsewhere in this report.) The second day Risø's benchmark program, Adina, was installed on the Paoli B7800, which is similar to the Risø B7800, and some test runs with the program were made. Time measurements indicated a much better performance than in the corresponding tests at Risø. It was agreed that Risø could get a copy of the current Paoli compiler with a view to try later to complete the Adina benchmark tests at Risø.

5.4. Completion of Benchmarking and Status Ultimo 1982

The compiler brought home from Paoli was two releases ahead of the remaining Burroughs system software at Risø; nevertheless, it was decided to install it as an experimental compiler. In doing this, many old errors were gone, but unfortunately a few new ones had entered. This impeded once more a successful completion of the Adina runs. After a telephone patch was received through Burroughs Denmark and installed, we finally succeeded with the Fortran 77 benchmarking.

By the end of 1982 a few compiler errors still remained. However, the error status has improved a lot during 1982, and much of this improvement has undoubtedly been triggered by Risø. Both the compile and runtime efficiency have improved and will probably still improve in the future. Present major obstacles are the unsolved linkage problems, which makes it virtually impossible to install a math library to support Fortran 77, and also the insufficient documentation standard. Indeed Burroughs has issued a Fortran 77 reference manual, but use of it is so far discouraged due to its many errors, its incompleteness, its obsolescence, and its lack of illustrative examples.

In November 1982, the Computer Installation arranged a programming course in Fortran 77, and at the same time Fortran 77 was released for general use at Risø. Apparently there is a pronounced interest among the users to benefit from the many enhancements in Fortran 77 compared to the old Fortran language. We have also noticed a growing number of Fortran 77 programs coming to Risø from outside.

6. WORKING ENVIRONMENT AND SECURITY

The purpose of the Danish working environment law is to obtain an acceptable working environment from the point of view of security and well being for all employees. To implement this a security group is formed within each work area. The security group consists of a work leader and a security representative, who is elected by and among the employees. Both group members must follow a full week course about working environment and security.

The security group has many tasks. It is concerned with the actual work situation, but it also takes part in the planning of the departmental activities. The group shall thus be involved in the planning of work routines, work processes, work methods and changes herein, the extensions or alterations of the department, procurement and changes of machinery and technical aids, and purchase and use of various items.

In the period of this report, the Computer Installation security group has had an unusual number of items of business, because of Risø's new EDP-installation set up in a new building.

From the very beginning the security group was brought into the planning of this building, in that the members of the group were the department's representatives in the building committee. Throughout the entire period the group was involved in the planning and organization of the structure. Despite the economic restrictions it was important to get a building that functioned and filled the demands and norms contained in the law of the work environment.

The result may be viewed as being satisfactory. We have acquired a suitably arranged building with an environment especially adapted to a computer installation in terms of noise, indoor climate, and lighting. This was achieved in different ways, for

example, with divided-up service- and non-service areas, sound insulation, stained glass areas, and low-level illumination fittings.

Apart from the work connected with the new building, the group attempted to make different terminal work places in the Computer Installation as acceptable as possible. Here the choice of terminals and terminal tables can be mentioned along with the setting up of low-level illumination fittings and the installation of sun curtains, all for the purpose of producing a good working environment and a good working place at the terminals.



Changing a disk-pack. Note sound-attenuating baffles under the ceiling

7. LIBRARY

Burroughs has introduced a new software feature called Library. Library is a program which provides a set of subroutine entry points which can be reached by other programs. A call on a procedure in a Library is equivalent to a call on a procedure (or a subroutine) in the user's program.

In Rise Computer Library we will use the Library feature to create Libraries in Algol and Fortran consisting of precompiled routines. Since the routines in a Fortran Library can be called not only from a Fortran program but also from an Algol one it is clear that we need not translate Fortran subroutines into Algol in the future in order to use them in an Algol program.

Here it must be emphasized that there are still some deficiencies in the Library, especially the Fortran Library. A Library in Fortran has at least two serious drawbacks. The first is that a parameter of a Library subroutine cannot itself be a subroutine. This prevents the installation of a complete mathematical subroutine library using the Library feature. Examples of subroutines which for the present must be omitted from a Library are: quadrature routines, differential equation solvers and minimization routines all of which have subroutine parameters.

A second drawback is that the user must supply the so-called "skeleton routines" which describe the routines' parameters in order to use the Library. This drawback is not prohibitive but only inconvenient since the skeleton routines can be supplied via a file of skeleton routines to be included by the user of the Library.

Regarding an Algol Library it is also necessary to supply skeleton routines but here no feeling of inconvenience is present because procedures in Algol always have to be declared according to the philosophy of that language.

But bearing in mind the necessity of skeleton routines we should like to have such routines declared automatically during the creation of a Library such that procedure and subroutine declarations belonging to a given Library are known to the user's program. This must be possible to implement because it is done for the intrinsics.

Regarding the use of Fortran Library in an Algol program - and the reverse - it has to be remarked that array parameters must be one-dimensional. A parameter referring to a two-dimensional array is inconvenient because it is thus necessary to transfer the content of the two-dimensional array to a one-dimensional one before the call of, say, a Fortran Library routine.

It is our hope that the drawbacks mentioned above will find a satisfactory solution in the near future.

In a similar way under some restrictions we can use precompiled Algol procedures in a Fortran program. We do this in RIPS (Rise Interactive Plotting System) which is designed for working with interactive graphic. The condition for mixing routines in different languages is that the routine parameters are of the same type.

The number of statistical routines in the Algol part of RCL has always been very small compared to the same chapter in the Fortran part. In order to be familiar with the Library feature we started on a project the goal of which was the creation of a Fortran Library containing the precompiled statistical subroutines from the Fortran part of RCL and which can be used by an Algol program.

The project was successfully finished at the end of 1982 and the experience gained will be useful in a forthcoming revision of RCL in both Algol and Fortran.

8. RECENT DEVELOPMENT IN RISO COMPUTER LIBRARY

The Riso Computer Library (RCL) has been maintained and further developed through the period. Some desired test programs and descriptions have been generated.

As a general rule test programs shall exist to all the routines in RCL. This rule has hitherto not been fulfilled for all routines obtained from outside Riso. The remaining test programs have now been implemented and the corresponding routines are tested once more.

When Riso's first computer, GIER, was replaced with B6700 in 1972 several Algol procedures were taken over to the Burroughs computer system, but with a syntax check only. Some of these procedures have later become obsolete, but the remaining routines have been tested on our new B7800 and their original descriptions belonging to the GIER epoch are transferred to the source text of the procedures in accordance with what are used for all other Algol procedures in RCL. All the Algol procedures in RCL are now at the same standard regarding their function as well as their description.

9. RISØ INTERACTIVE PLOTTING SYSTEM

Since RIPS (Risø Interactive Plotting System) was released in August 1980 it has turned out that the fundamental assumptions made when developing the system were true, and more and more users have found it worthwhile to implement their plotting programs by using this system.

The plotters at the central computer installation practically never pause and due to the interactivity in the system the drawings are of a very high quality.

9.1. RIPS as a Library

One of the main objections to the system in the beginning was the compilation time. The initial system was included in the user's program as Algol-statements (about 7 000 lines) and had to be compiled every time, producing a great overhead in program development. Fortunately we got a new software tool, the Library concept, by which all the routines in the system can be compiled once and then linked to the user's programs at runtime. This reduced the compilation time for the user from about 30 sec to about 1.5 sec.

When the RIPS-Library is running, it fully controls all the parameters describing the user's coordinate-system, devices, etc. The user has no direct access to these parameters and can change the values only via routines in the Library. In this way the routine environment is preserved and the Library alone is responsible for the system's integrity.

Another advantage of the Library concept is that fundamental changes in a system like RIPS take immediate effect in all programs using the system without any recompilation of the users' programs. The routines in the Library are not linked to the

program until runtime and thus it is the newest version of the Library with all the changes that is running. This gives a very flexible and easy way of changing the system without disturbing the users.

9.2. RIPS in Fortran

The RIPS-Library is programmed in Algol, but as it contains all the describing parameters itself and can be called from programs written in other languages than Algol, it was not very difficult to implement RIPS in Fortran.

One of the major advantages in RIPS is the notion of an Image as a datatype containing the description of a picture. In Algol the datatype String is used to hold this datatype. Fortran has no such variables and therefore it cannot manipulate Image's directly. Instead the RIPS-Library maintains an Image-variable which at all times contains the picture created by the user, and by the use of subroutines the Fortran user has control over this Image.

In this way a fully functional system has been established, and as the interactive module, Imagehandler, is the same as in Algol, the interactive facilities are now fully available in Fortran.

10. THE TEXT-EDITING SYSTEM SETUP

Although dedicated text-editing systems have become more common at Risø during the last two years, Setup has been used extensively since its release. However, it is obvious that it will lose in the competition with dedicated text-editing systems, unless substantial resources are allocated to an improvement of Setup. Three major improvements seem to be of importance:

- 1) more flexible editor to handle the draft,
- 2) better facilities for writing formulas (Greek letters super/suffix etc.), and an
- 3) output to phototyping equipment.

The following facilities have been added to Setup since its first release:

- 1) tabulate mode, a convenient tool for setting up tables,
- 2) Contents, a tool for automatic creation of contents with page references,
- 3) Index, a tool for automatic creation of a keyword-list with page references, and
- 4) several minor features and corrections of most of the known faults.

11. REDUCE - AN ALGEBRAIC PROGRAMMING SYSTEM IMPLEMENTED ON RISØ'S B7800 COMPUTER

Today it is possible in some fields for people with time-consuming algebraic calculations on their hands to use a computer program for that purpose. And the fields in which these techniques are being used are so diverse that there seems every prospect that computer algebra will spread.

If the objective of computerizing algebra is to provide mathematicians, physicists, and engineers with an algebraic assistant, the computer systems must be versatile. This consideration underlies the attempts which have been made in the late 1960's and early 1970's to develop general-purpose algebraic computer programs, the best known of which is called Macsyma, used at the Massachusetts Institute of Technology. A similar computer system called Reduce was developed during the same period at the University of Utah. In principle these programs are designed to deal with whatever algebraic problems may be thrown at them.

The Reduce system was largely developed by A. C. Hearn and is written in a dialect of the computer language Lisp. Its capabilities include:

- 1) expansion and ordering of polynomials and rational functions,
- 2) symbolic differentiations,
- 3) substitutions and pattern matching in a wide variety of forms,
- 4) calculation of the greatest common divisor of two polynomials,

- 5) automatic and user-controlled simplification of expressions,
- 6) calculations with symbolic matrices,
- 7) a complete language (Lisp) for symbolic calculations, in which the Reduce program itself is written,
- 8) calculations in high-energy physics, and
- 9) tensor operations.

The Reduce system for the B7000/B6000 series consists of four parts: the Reduce algebraic processor itself, a Lisp processor, a Lisp compiler which converts Lisp programs to an intermediate language, and an assembler which converts the intermediate language to Burroughs Algol.

The algebraic processor, the computer and the assembler are written in Rlisp, a sort of Lisp with Algol-like syntax. The Lisp processor is written partly in Algol and partly in Rlisp. All these parts are combined into a single large Algol program. The parts written in Rlisp must first be translated into Algol accomplished by the algebraic processor.

This Reduce system, supplied unofficially by Burroughs, has been implemented at the Risø B7800 computer. In order to facilitate the use of the system, it has been made a Cande-utility program by means of a locally written driver. The default option thus is input from the workfile and output to a program-generated diskfile. However, various input and output options are available.

At the time of writing the Reduce system has been in use only a few months. However, it has already been used for several applications mainly in the fields of differentiations and matrix manipulations.

12. IMPROVED DISKALLOCATION ALGORITHM

The standard diskallocation algorithm is essentially a best-fit algorithm, and most standard software defines a diskarea module with the same fixed size. The basic idea is that when a diskarea is released, the available space will provide a perfect fit for the next allocation of a diskarea-module.

However, to save disk space by releasing the unused part of the last diskarea in a file, the option of closing a file with crunch is also a standard feature.

The negative effects of crunching a diskarea-module is that the released area is less than the module size and cannot be used for allocating another diskarea-module. Furthermore, the inuse part of the diskarea is no longer allocated in a best-fit location on the disk.

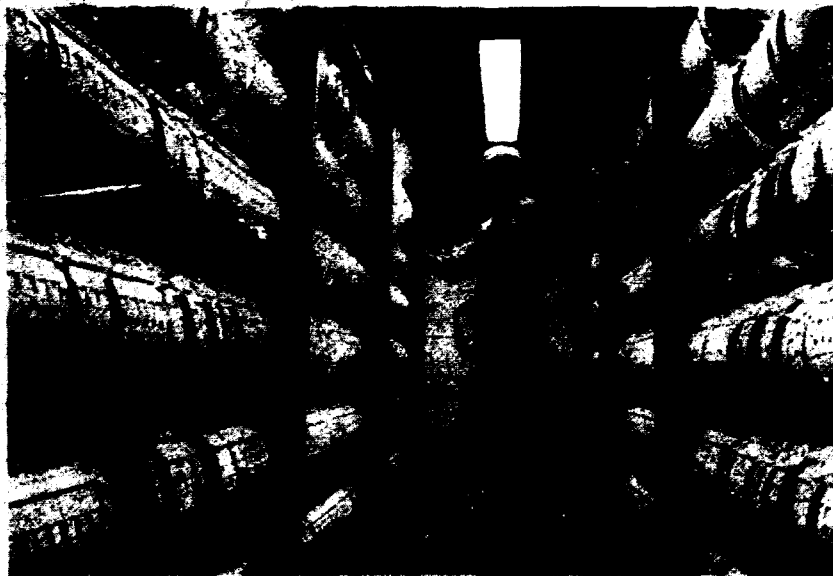
The available space on the disk will rapidly be scattered into a lot of small fragments of crunched diskarea-residuals, which are too small to contain a full module. And though a lot of disk space is released by crunching files, the available areas may be wasted anyhow.

We have modified these standard algorithms, so that crunching a file will reallocate the inuse part of the diskarea (whenever possible) to a best-fit location. On successful completion of the reallocation, the original diskarea is released as available space.

This change has the double effect of utilizing any small available areas for reallocations of small inuse parts, and it releases areas large enough to contain full diskarea-modules.

Our measurements on the effect of the improved algorithm confirmed its correctness. By the time of installation of the

change, the sum of available areas less than the standard disk-area module size was 90 Megabyte on a 600 Megabyte disk with 500 Megabyte inuse disk space. After 10 days of operation this amount was reduced to 30 Megabyte. We do not have any measures of the amount of crunching and reallocations, but the measured disk is the central secondary storage medium in the installation, which is undoubtedly the most dynamically updated disk. If removal of files could have been avoided in the period of measurement the resulting amount of scattered available disk areas would probably have been close to zero.



The tape library

13. DIVISION OF COMPLEX NUMBERS

During the installation and test of Eispack, a package for linear eigenvalue problems, we found that the use of the Burroughs intrinsic for complex division sometimes resulted in a division by zero because of an unnecessary underflow. An examination of the code for this intrinsic showed that it was a direct implementation of the arithmetic expression for the complex division such as it is known from ordinary high school books in elementary mathematics. No action was taken in order to avoid underflow.

A new complex division routine which included scaling in order to avoid under- and overflow was written by one of the staff members and included in our local B7800 system instead of the original Burroughs version. A copy of the complex division routine was also sent to the Burroughs compiler group as a proposal for a new intrinsic.

In their reply the Burroughs compiler group notified that even though our code was a better one, numerical noise could take place in the imaginary part of the result as an effect of the scaling. This was demonstrated by an example. Because of that Burroughs could not accept our proposal and therefore they made their own code which uses double precision division in order to avoid under- or overflow and scaling problems. A copy of the code was tested on our B7800 with correct results, but with very long executing times, 150 microseconds for a complex division.

We could not accept the solution presented by Burroughs because we have experienced that division in double precision is much more costly on B7800 than on B6700. Tests show that a double-precision division is 7-10 times slower than a single one.

We therefore reconsidered the problem and wrote a roundoff-free single-precision scaled complex division routine. The scaling is made as shifts in the octal exponent fields thus preserving the precision and the code will give no premature under- or overflow. Tests show that our last code is 3 times faster than the last proposal by Burroughs, i.e. a complex division in single precision takes 50 microseconds.



Output delivery

14. TRAINING ACTIVITIES

In the period under review in this report, the Computer Installation has carried through an extended programme of courses and colloquia about data processing matters for Risø personnel. We have also arranged a few courses with speakers from other departments or with speakers, external to Risø.

Several reasons provided the impetus for a major effort in this area in autumn 1981. Firstly, training had been neglected in the previous period due to the work with evaluation of proposals for a new computer. Secondly, systems work and developments would be limited in the remaining part of the B6700-period. And due to the heavy load on that computer, the users would be well motivated to increase their knowledge in order to improve their programs.

We decided to give many short courses rather than few extended ones, as we thought that this would more easily fit the working schedules of the participants, e.g. instead of one course in extended Algol, we offered six half-day courses in debugging, pointers, sorting, etc.

In total, we produced a list of 28 possible courses and sent it to the users. We picked two fundamental courses to be given every half year. They were "Introduction to The Computer Installation" and "Cande" (the terminal language). Both aim at helping a new user who knows about programming of other computers from earlier jobs or formal education.

The next six courses were also chosen by ourselves, but after that the scheduling of the different courses has mainly been decided by the number of preliminary registrations we receive from the users.

In the autumn of 1981, we gave eleven different courses in twelve weeks. Further, two of these were repeated due to over-booking. The spring 1982 included ten courses plus one da capo, and in the autumn '82, we reduced the number to eight, two of which were given by the staffs of NEUCC and RECKU, the Computer Installations of The Technical University and Copenhagen University, respectively. A revised list of possible courses had 32 entries.

As a part of this work, some instructional material and a number of manuals or guides have been written or revised. We believe that our training activity now has settled at a level which we can support permanently and which is well adjusted to the needs of our users.

The benefits are hopefully better knowledge among the users of available tools and methods, more efficient use of the computer, and improved contact between the users and the staff of the Computer Installation.



Advice to a user

15. FORMATION CONSTANTS IN CHEMICAL EQUILIBRIUM REACTIONS

In 1981 the Computer Installation participated in a contract enterprise of the Chemical Department on research tools for determining the formation constants in complex equilibrium reactions. The experimental techniques are spectrophotometrical measurements of a number (s) of prepared chemical solutions, recorded for a set of w selected wavelengths. In this way an s -by- w data matrix D is obtained. The goal of the analysis is to infer from D how many reaction constants (c) should be assumed to exist for a given chemical system, and to calculate their values. This problem was solved by a combination of factor analysis and optimization techniques. The idea is to approximate D by a matrix product CE , where the s -by- c matrix C contains the concentrations in each solution of each of the postulated c reaction components, and the elements of the c -by- w matrix E are the molar extinctions at the given wavelengths. Thus we assume that $CE = D + R$ where R is expected to be a small residual matrix. To assess c we followed the standard practice in factor analysis and computed the eigenvalues of the symmetric matrix $A = D(T)D$ and let c be the 'effective rank' of A . The actual computations were performed by aid of the so-called singular-value-decomposition (SVD) of D . Having decided a value of c we next faced the problem of estimating the elements of the constituent factors C and E . Let k be the $(c-1)$ -vector of formation constants in the chemical system. When k is given you can compute C from the reaction equations and the assumed nature of the system considered; hence we can write $C = C(k)$. We intend to compute the 'best' k in some reasonable sense. The approach we held to was to solve the following double minimization problem:

$$\min_k \left(\min_{E \text{ nonnegative}} \text{norm of } (C(k) E - D) \right)$$

Here the Euclidean norm is used; its square is just the sum of the squares of all the matrix elements. Let us first discuss

the inner minimization problem. The vector k is here considered as fixed, and so is $C(k)$. Determination of the matrix E that minimizes the norm of the residual matrix $R = CE - D$ is equivalent to the solution of w linear least-squares problems, one for each of the wavelengths. The solution of these subproblems would be trivial, if not for the constraint of nonnegative E . With this constraint present the problem is a special case of a quadratical programming (QP) problem. A code was written to solve this QP; the solution method utilizes Lemke's simplex-like algorithm based on the principle of complementary slacks (by the way, this QP code was later used to solve a nuclear cross-section fitting problem in the Department of Energy Technology.) Having solved the inner minimization problem, the devised procedure may be used as a subordinate algorithm in the outer minimization process, in which the components of k , that is the reaction constants, are estimated. This job was done by a standard algorithm for unconstrained minimization of a sum of squares as a function of nonlinear parameters. The algorithm, which is of the Levenberg-Marquardt type, was taken from the program collection Minpack1, an optimization package developed in Argonne National Lab., USA.

Some graphical tools were also applied in the project. First, the original data matrix D could be depicted as a contour map to give a rough idea of what the data look like. Secondly, the computed extinction spectra could be drawn using spline interpolation.

By means of the computational analysis outlined it was possible to identify reaction constants for synthetic as well as real measured absorption spectra from various types of complex reactions.

16. MATHEMATICAL MODEL FOR ATMOSPHERIC TURBULENCE

Since the autumn of 1981 the Computer Installation has cooperated with the Meteorology Section at Risø on the development of a mathematical model for turbulent flows in the atmosphere. Also NCAR (National Center for Atmospheric Research) in USA has contributed to this work, which is described in "Risø Report No. 478: Squashed Atmospheric Turbulence", by Leif Kristensen, Peter Kirkegaard, and Donald Lenschow (to appear in 1983.) The final outcome of the project was coordinated during two meetings among the three authors, the first held at Risø in March 1982, the second at NCAR in October of the same year.

The actual model is kinematical and of the second order, valid for axisymmetric, nearly isotropic turbulence. The spectral tensor contains three scalar functions of the wave number magnitude. In principle, these can be determined from one-point experimental velocity spectra by solving two integral equations of the Volterra type, which include these spectra in the source terms. Explicit solutions were found under rather general circumstances without specifying the analytical forms of the component spectra. Velocity component spectra with vertical wave numbers and lateral and vertical spectral coherences were derived. With rather general assumptions about the analytical forms of the velocity spectra (with horizontal wave numbers and a vertical symmetry axis of rotation) the spectral tensor can be obtained in terms of known functions. Those velocity spectra contain five parameters, which can be extracted from spectral characteristics of the convective boundary layer.

The contribution from the Computer Installation to this work was in the first place to devise an analytical method for solving the integral equations; this led to a breakthrough in the development of the model. It also comprised coding of the model as the Fortran program Axisym, which was implemented both at the B7800 at Risø and a VAX-11/780 computer at NCAR. Numerical as-

pects of the coding included the construction of a subroutine for the incomplete beta function valid beyond the domain of parameters where the function can be normalized, as well as integration methods suitable for computation of the spectral coherences, these being infinite integrals of oscillating functions. Many of the formulas emerging from the model were quite complicated and cumbersome to deduce. The symbolic-algebra system Reduce (described elsewhere in this report) was used to a wide extent for checking of the formulas. Unfortunately, we could not benefit from Reduce in the constructive part of the work, as the system by then was not yet installed. Several graphical tools were applied in Axisym; apart from locally developed plotting software we used the system Redips (= Risø Engineering Department Interactive Plotting System) for construction of perspective surface plots.

In a forthcoming project it is planned to infer the five spectral parameters from experimental data. This will be accomplished through the use of fitting and approximation methods.

17. USERPROGRAMMER

A new position as a userprogrammer in the Computer Installation was opened early 1981.

The purpose of this new position is that the Computer Installation shall be able to offer programming help to those departments at Risø that have no trained EDP-personnel available themselves. The position was filled in late June and the balance of the year was used for training and closed with the working out of an addition to the text-editing program Setup.

In January 1982 the offer to provide assistance in programming was announced, and during the year the Computer Installation rendered aid to the Physics and Chemistry Departments as well as the Isotope Laboratory.

The Physics Department requested assistance first, as it wished to put its files of climatic data measurements covering the years 1958-82 in order. The measurements were taken with different time intervals: one hour during the 1958-71 period and ten minutes during 1972-82. The files, typically containing one year's measurements, were arranged in different ways and on different media, making the work rather troublesome. In order to simplify the effort it was decided to collect all measurements from 1958-82 on a diskpack, with one-hour intervals between each, and organized in a way such that the work may proceed with the help of the Cande program.

Next a project for the Chemistry Department's radical group was started. The work was defined as a renovation of an existing program for treating experimental measurement data, which consisted of digitized lifetime curves for short-lived molecular fragments (free radicals) that are formed by pulse radiolysis combined with kinetic spectroscopy.

However, it soon became obvious that it could be worthwhile to start completely from the ground up and construct a command-managed program as a replacement of the existing dialog program. Even if a large part of the previous work must indeed be given up, certain advantages in the use of commands are immediately evident, specifically an improved structure and larger flexibility, which facilitate the incorporation of new ideas arising from the development of the program.

In the autumn, the Isotope Laboratory came up with a wish for two programs. Here curves should be plotted showing, for example, the amount of different materials contained in old coins that the Danish National Museum had acquired. One of the programs should run as batch, while the other should be interactive with more possibilities for the manipulation of data than was the case with the first program. One thing that came out of the Chemistry Department experience was the decision to make a command-managed program which was then applicable here. This work was finished in December 1982.

18. SCANNET'S CONNECTION TO B7800

Since early 1980 Risø Library has been responsible for collecting abstracts of energy literature from the Scandinavian countries.

The data are edited on B7800 (previously B6700) after being entered from time-sharing terminals. Initially, the public telephone net was used to connect the Scandinavian libraries to the computer. In September 1980 it was decided to use Scannet to connect the terminals to the computer, with the following topology of the net. From B6700 the net appeared as a multidrop TD-830 line with 6 terminals. This line enters a NORD-12 computer sited at the National Technological Library of Denmark near Copenhagen. The NORD-12 simulates the 6 TD-830 terminals and retransmits the data to a concentrator at the Danish Telephone Headquarters in Copenhagen. The concentrator is connected to those of the other Scandinavian countries. The actual users of the net - using TTY-compatible equipment - dial in to one of these concentrators.

The actual implementation of the attachment of B6700 to the net was made by Risø as far as the B6700 is concerned and by Scannet as far as the NORD-12 is concerned.

The person in charge of the NORD-12 was sited in Stockholm, where the software development equipment was placed. This implied that most patches had to be created in Stockholm and then transported to Copenhagen where they were checked out against B6700. This inadequate logistic obviously created extreme delays.

The Scannet was taken into use for this purpose in the autumn of 1981 although it had several shortcomings, e.g. output from the computer to a terminal could not be stopped by the break-function. The connection was actually not fully operational be-

fore late 1982. The complex structure and the ill-defined responsibility still create difficulties in the maintenance of the net.

However, medio 1982 plans came up to eliminate Scannet, so now the work is going on with a change from Scannet to the public data-net.

This project has been an organisational and functional demonstration of poor management.

19. MULTIPLE QUADRATURE

The study in this area has been continued. Attempts have been made to find a method which can construct symmetric non-product formulas with positive quadrature weights in a systematic way, where both the number of quadrature points is as small as possible and the fraction of reusable quadrature points as large as possible.

This goal has not been attained but with an experimental program designed for the purpose it has been possible to find quadrature formulas for hypercubes up to dimension 6 and order 6 with the desired properties.

APPENDIX A

CONFIGURATION OF THE RISØ B7800 COMPUTER AS OF DECEMBER 1982

- 2 Central Processor Module, 8 MHz.
- 1 Input-Output Module with 28 Channels.
- 768 K Storage, 48 data bit plus 3 tag bit plus 9 parity bit.
- 1 Maintenance Processor (B800) with Console and Magnetic Tape Station.
- 2 Dual Disk Drive (Fixed, Model 207)/Dual Controller with a total of 800 MB.
- 2 Dual Disk Drive (Exchangeable, Model 225)/Dual Controller with a total of 4 x 87.2 MB.
- 3 Magnetic Tape Drives, 9 track, 800/1600 bpi, 100/200 KB/s.
- 1 Card Reader, 800 cards/minute.
- 1 Card Punch, 100 cards/minute.
- 1 Line Printer, 132 printpositions, 64 characters, 1100 lines/minute.
- 2 Calcomp 507/565 Digital Plotters.
- 1 Calcomp 1012 Digital Plotter.
- 3 Operator Console Displays.
- 1 Data Communication Processor, 8 K local storage.
- 18 Line Adapters with Dial-up 300 baud Modems for Visual Display Units and Printing Terminals.
- 5 Line Adapters with Dial-up 1200 bit/s Modems for Graphic Terminals and Dataloggers.
- 5 Line Adapters with permanent connection to VDU's.
- 3 Line Adapters with locally built interfaces for Calcomp Plotters.
- 2 Line Adapters with permanent connection to PDP Mini-computers.
- 1 Line Adapter with permanent connection to a Remote Job Entry Terminal.
- 1 Line Adapter with permanent connection to a Remote Printer.

- 1 Line Adapter with permanent connection to a Nixdorf
 Computer (Risø's system for economic control).
- 1 Line Adapter with permanent connection to Scannet.
- 1 Line Adapter with Datel 2400 Modem for external computers.

TERMINAL EQUIPMENT AT THE COMPUTER INSTALLATION AS OF DECEMBER 1982.

- 4 TEC 610 Visual Display Units.**
- 2 Tandberg TDV 2220 Visual Display Units.**
- 1 Tektronix 4010-1 Graphical Terminal.**
- 1 Diablo 1620 KSR Printing Terminal.**
- 1 Diablo 1650 KSR Printing Terminal.**
- 1 Data Dynamic 303 KSR Printing Terminal.**
- 1 Centronics 6080 Lineprinter.**
- 1 PDP-8 Minicomputer with two Floppy Disk Drives, VDU,
Paper Tape Reader, Paper Tape Punch, 3M Cartridge Station
(ECMA 46), and Philips Cassette Tape Drive (ECMA 34).**

APPENDIX B

STAFF OF THE COMPUTER INSTALLATION 1 JANUARY 81 - 31 DECEMBER 82

Head: L. Hansson

Office staff: L. Hansen
H. Sørensen*
M. Høeg*

Scientific staff: E. Hansen
J. Houmann (from 1 August 1982)
P. Kirkegaard
O. Lang Rasmussen
P. Voss (until 31 May 1981)

Technical staff: C. Bergmann
S. Bechmann (from 1 September 1981)
H. Bundgård (until 28 February 1982)
J. Deutschbein
I. Elmholdt-Hansen
S. Frederiksen
T. Hansen (until 31 August 1981)
H. Kiærulf Kristensen
P. Lou (from 1 March 1982)
S. Madsen (from 22 June 1981)
S. Rahbek Petersen

* Temporary assistant

APPENDIX C

PRODUCTION STATISTICS 1981

	Production	On-line	PM	UM	Processor
January	417.40	1788.44	28.00	1.00	353.27
February	335.50	1819.21	31.00	10.55	259.02
March	395.35	1927.19	41.00		338.37
April	358.00	1435.23	23.00	16.00	327.20
May	334.35	1549.14	30.30	3.45	330.00
June	338.30	1570.22	30.40	7.50	380.00
July	440.45	1993.10	13.00		523.00
August	383.35	2025.06	31.00		389.00
September	405.25	1969.57	34.05	5.05	369.45
October	377.20	1729.37	19.15	31.25	343.25
November	418.40	1904.15	7.00	8.45	464.41
December	332.45	1935.02	21.00		457.46

Production: Hours and minutes the computer has been on for production runs.

On-line: Sum of use of terminals, hours and minutes.

PM: Preventive Maintenance, hours and minutes.

UM: Unforeseen Maintenance including waiting time, hours and minutes.

Processor: Automatically logged use of central processor, hours and minutes.

APPENDIX D

PRODUCTION STATISTICS 1982

	Production	On-line	PM	UM	Processor
B6700					
January	367.55	2266.17	20.40	2.30	436.17
February	352.30	2356.56	18.30	0.45	367.06
March	471.55	2583.52	27.15	1.30	479.23
April	407.20	2242.34	21.00	3.30	474.29
May	400.35	2246.14			539.48
June	260.20	1273.02			307.07
B7800					
June	116.35	1033.20			55.25
July	267.20	2257.14	14.00	4.20	162.33
August	263.20	2323.20	22.00	1.30	163.13
September	262.20	2503.17	10.00	5.00	166.49
October	247.15	2385.03	6.00	4.10	175.58
November	252.50	2921.35	10.15	5.10	191.02
December	239.50	2524.42	10.00		232.18

Production: Hours and minutes the computer has been on for production runs.

On-line: Sum of use of terminals, hours and minutes.

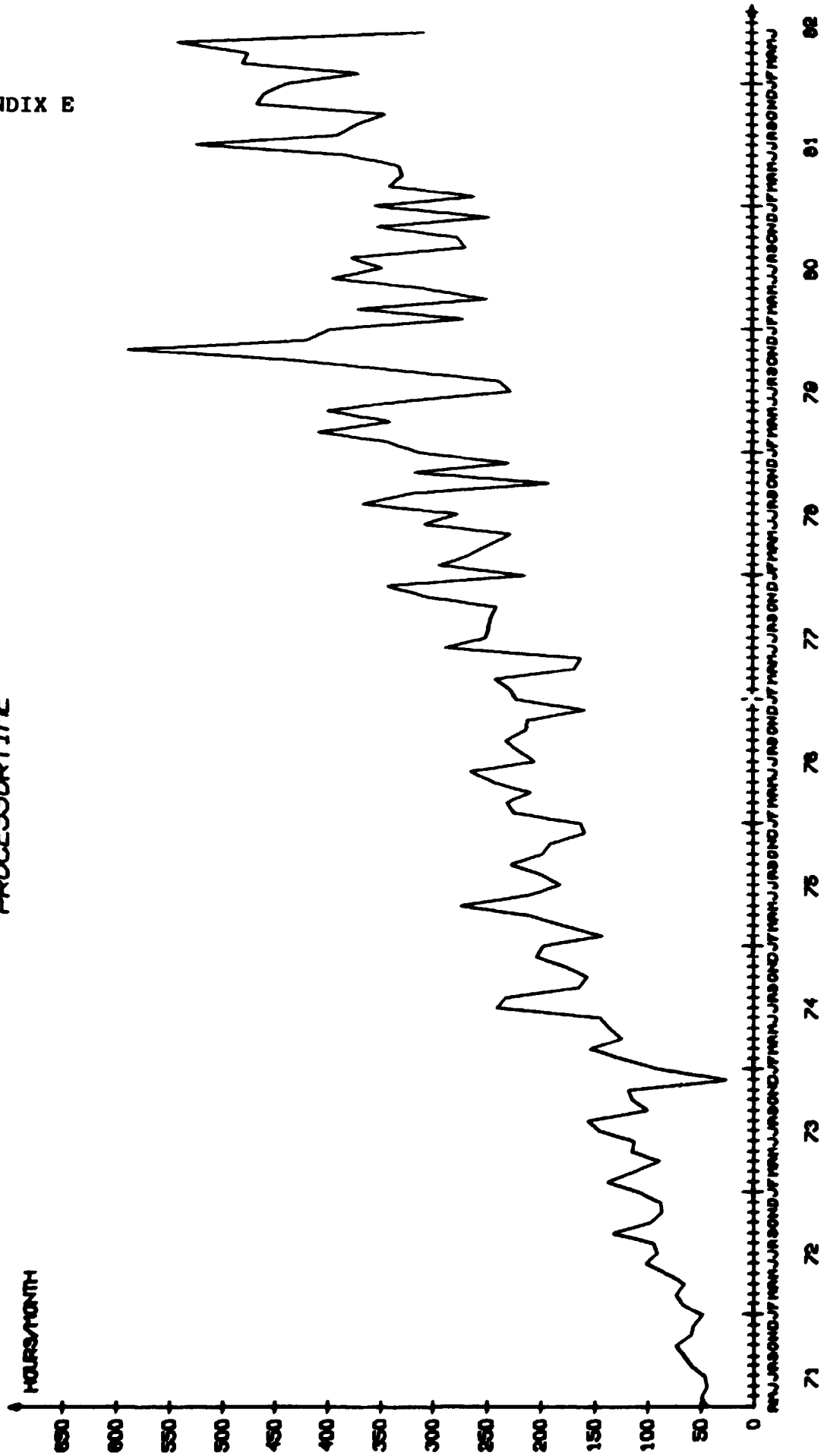
PM: Preventive Maintenance, hours and minutes.

UM: Unforeseen Maintenance including waiting time, hours and minutes.

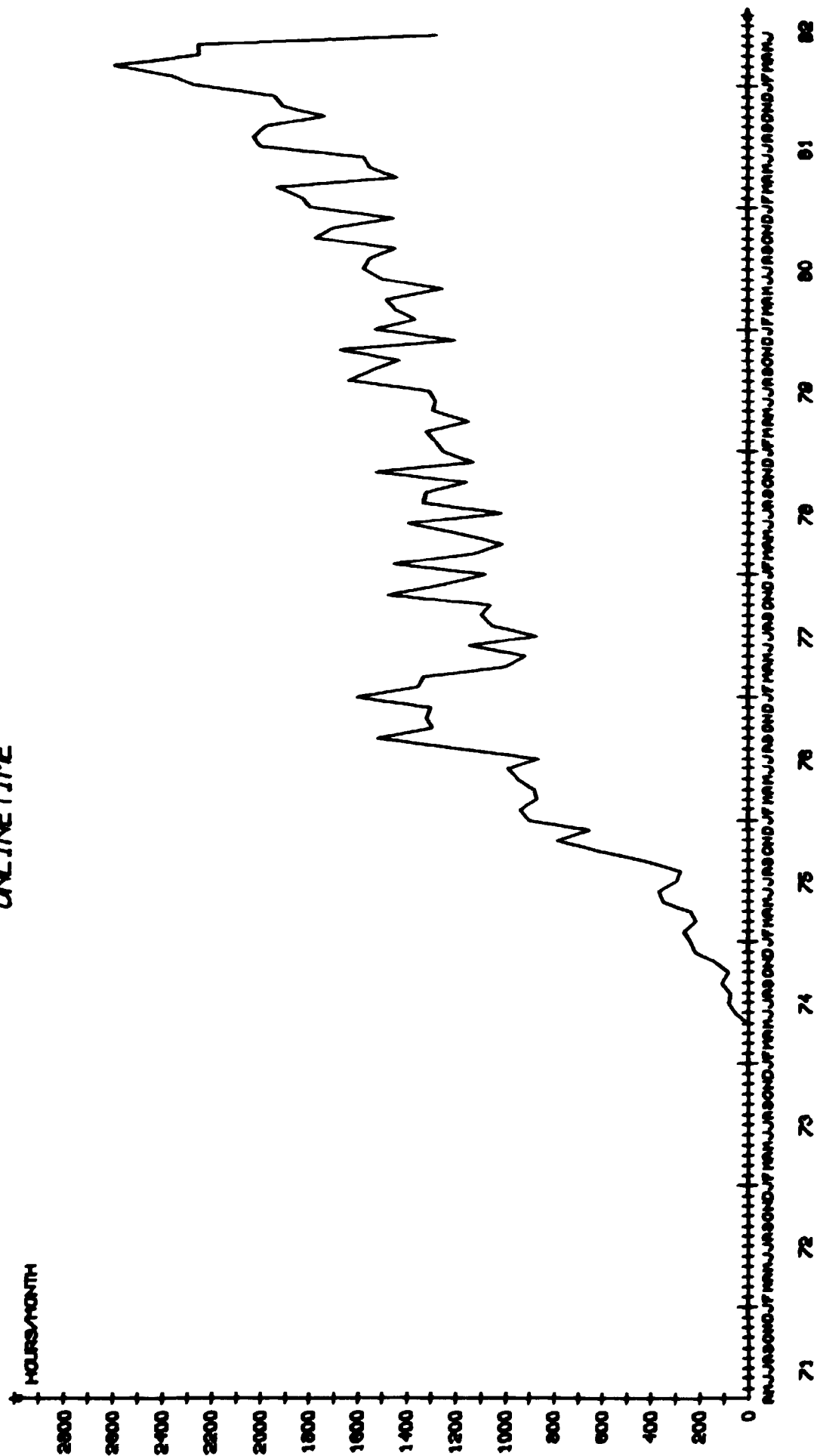
Processor: Automatically logged use of central processor, hours and minutes.

APPENDIX E

STATISTICS OF THE USE OF B6700.
PROCESSOR TIME



STATISTICS OF THE USE OF B6700. ONLINE TIME



2374

Risø - M -

<p>Title and author(s)</p> <p>PROGRESS REPORT 1 JANUARY 1981 - 31 DECEMBER 1982 COMPUTER INSTALLATION</p> <p>Leif Hansson</p>	<p>Date May 1983</p>
	<p>Department or group</p>
	<p>Group's own registration number(s)</p>
<p>53 pages + tables + illustrations</p>	<p>Copies to</p>
<p>Abstract</p> <p>This report describes selected parts of the activities at the Computer Installation of Risø National Laboratory in 1981 and 1982. Information given may be preliminary.</p> <p>Available on request from Risø Library, Risø National Laboratory (Risø Bibliotek), Forsøgsanlæg Risø), DK-4000 Roskilde, Denmark Telephone: (02) 37 12 12, ext. 2262. Telex: 43116</p>	